

# Low-temperature dynamics of spin glasses: Walking in the energy landscape

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## Abstract

We analyse the relationship between dynamics and configuration space structure of Ising spin glass systems. The exact knowledge of the structure of the low-energy landscape is used to study the relaxation of the system by random walk in the configuration space. The influence of the size of the valleys, clusters and energy barriers and the connectivity between them on the spin correlation function is shown.

*Key words:* Spin glass; Energy landscape; Relaxation; Computer simulations

*PACS:* 75.50.Lk, 75.10.Nr, 61.20.Lc

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## 1 Introduction

In general, systems which comprehend disorder and competing interactions (frustration) are characterised by a complex landscape in the high dimensional configuration space. The dynamics of such systems is strongly correlated with their complex topography of the phase space. Consequently, dynamical processes are determined by the movement in the space. The strong increase of the relaxation time for low temperatures is related to metastable states and global minima acting as basins of attractions. It has been established that the underlying mechanism is uniform for different systems, e.g. spin glasses, supercooled liquids and the protein folding problem. The physical understanding of the behaviour of these systems from a microscopic point of view is a major challenge. It would demand the knowledge of the huge number of system states, the connectivity of these states in the configuration space and their correlation with real space properties. Numerical investigations are restricted

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to small systems and various procedures are proposed, e.g., molecular dynamics simulation presented for supercooled liquids (1; 2), pocket analysis of the phase space around a local minima (3), and random walk in the energy landscape of spin glasses (4; 5). In this work we calculate the exact low-energy landscape for a finite spin glass system and study the dynamics by a random walk through the configuration space.

## 2 Model and landscape

The system is described by the Hamiltonian

$$H = - \sum_{i < j} J_{ij} S_i S_j \quad (1)$$

on the simple cubic lattice with periodic boundary conditions. The sum runs over all nearest neighbour pairs of Ising spins  $S_i$  with values  $\pm 1$ . The sample is prepared by randomly assigning exchange couplings  $J_{ij} = \pm J$  to the bonds of the lattice. In this paper only one specific random arrangement of exchange couplings  $\{J_{ij}\}$  for a finite system of the size  $N = 4 \times 4 \times 4$  is used. All 1635796 states up to the third excitation were calculated using the branch-and-bound method of discrete optimisation (6). The schematic picture of the configuration space is visualised in Fig. 1. It forms an energy landscape consisting of clusters, valleys and barriers. A set of configurations is called a cluster, if a “chain” exists connecting them. The chain is built up by neighbouring configurations, where neighbours are states of the same energy, which differ in the orientation of one spin. The landscape is symmetrical due to Eq. (1). Two clusters of different energies are connected whenever at least one configuration of the first cluster differs from one configuration of the second cluster by only a one-spin flip. The two different ground state clusters #1 and #2, e.g., consist of 12 and 18 configurations, respectively. Valleys can be assigned to these ground state clusters. A valley puts together all clusters, which only have connections with its ground state cluster. Different valleys are connected by so-called saddle clusters, which procure the transition over energy barriers.

## 3 Method and dynamics

The complete knowledge of the low-energy landscape allows us to investigate the influence of the size and structure of clusters and valleys and their connectivity on the dynamics. The time evolution of the system in the configuration

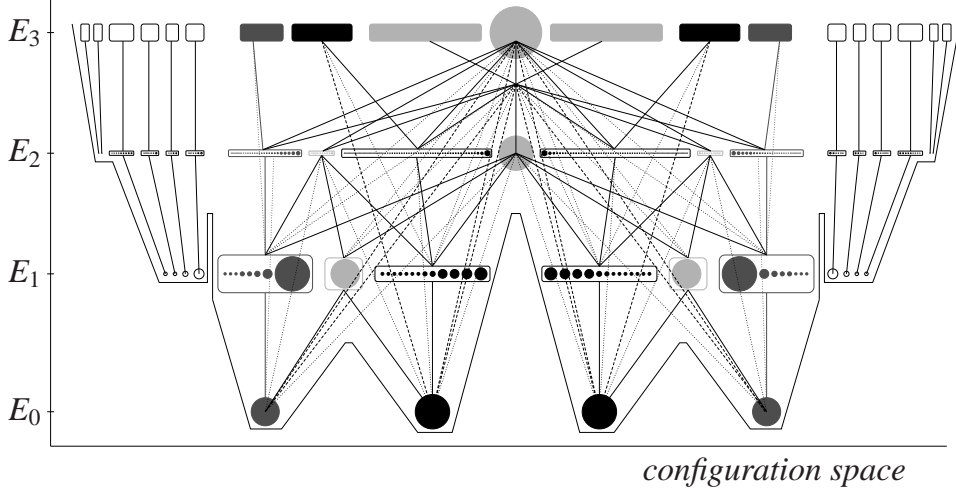


Fig. 1. Schematic picture of the exact low-energy landscape up to the third excitation. Clusters are marked by circles, where the size is proportional to the number of configurations in the cluster (note that the scale is different for different energy levels: the largest cluster in the first, second and third excitation contains 819, 82960 and 1503690, respectively). The lines denote the one-spin flip connections. All clusters with the same connectivity are pooled by a box.

space can be described as the progressive exploration of clusters and valleys. We use the Monte Carlo Metropolis algorithm for different  $\beta = (k_B T)^{-1}$ , where  $T$  is the temperature of the heat bath (7). One Monte Carlo step (MCS) is used as time unit. An individual run through the landscape is shown in Fig. 2. We start from an arbitrary state in the left ground state cluster (#1) of Fig. 1. First the system walks in the valley and sometimes touches the saddle cluster in the first excitation. After an escape time  $t_{esc}$  in the order of  $10^7$  MCS the system leaves the first valley and goes through the saddle cluster

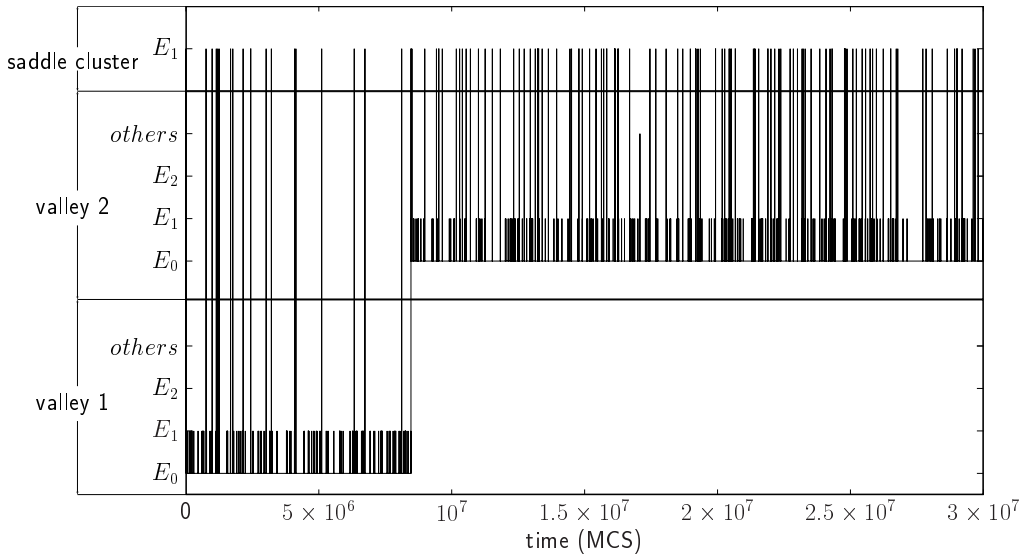


Fig. 2. An individual run through the landscape vs. time ( $\beta = 2.5$ ).

to the second one. This transition is determined by the internal structure of the saddle cluster shown as its transition profile in Fig. 3. First all pairs of configurations are checked to find out the largest hamming distance  $h_d$  ( $h_d$  of a spin pair is one half of the difference of the sum over all spins). Then one of these both states is used as reference state and the  $h_d$  values of all configurations of the saddle cluster with respect to this reference state are calculated. Two sets of states, which have one-spin-flip connection with the ground states of both affiliated valleys, are marked. They denote the input and the output area for a transition from the first valley (#1) to the second one (#2). Obviously, a transition as a walking between these sets is slowed down due to the smaller numbers of states between.

Quantitatively, the random walk can be described by the spin correlation function

$$q(t) = \frac{1}{N} \langle S_i^G(0) S_i(t) \rangle, \quad (2)$$

where  $S_i^G(0)$  is the  $i$ -th spin of the starting configuration arbitrary chosen from the ground states of valley #1 (#2). The brackets denote the average over 100 runs starting from the same state (Fig. 4).

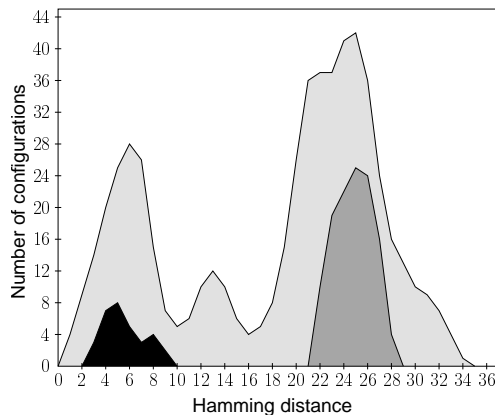


Fig. 3. The transition profile of the saddle cluster illustrated by the number of configurations vs. hamming distance from a reference state (see text). The shaded area marks all configuration in the saddle cluster. States having connections with the valley #1 (dark) and #2 (middle) are specially emphasised.

## 4 Results and discussion

The spin correlation function vs. time is characterised by a plateau with the value  $q_{pl}$  followed by a temperature dependent decay. To examine the correlation between the structure of the landscape and the dynamics we compare  $q_{pl}$  with the size of the valley having in mind that the spin correlation within

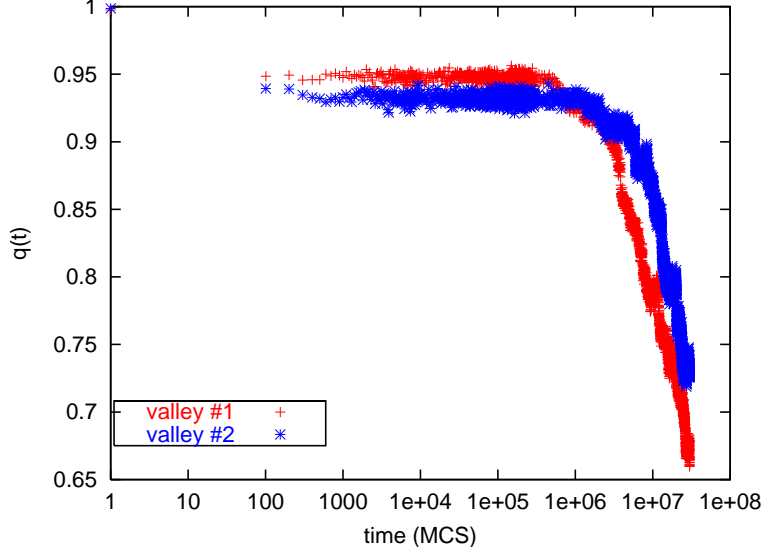


Fig. 4. The spin correlation function vs. time. The starting configuration is selected from the set of ground states of valley #1 and #2 ( $\beta = 2.5$ ).

the valley can be calculated using the mean hamming distance  $\bar{h}_d$  of all pairs of states by

$$q_{pl}^{(ham)} = 1 - 2\bar{h}_d/N. \quad (3)$$

We found an agreement between  $q_{pl}$  and  $q_{pl}^{(ham)}$  (Table 1), where the average in Eq. (3) is performed over all states in the ground state cluster. So the plateau reflects the dynamics within the valley.

The subsequent decay of  $q(t)$  shows the escape from the valley. The escape time  $t_{esc}$  depends on the temperature and can be fitted by  $t_{esc} \sim \exp(\beta \Delta E_{eff})$ . We found  $\Delta E_{eff} = 4.24 \pm 0.08$  ( $4.46 \pm 0.09$ ) for valley #1 (#2), respectively. Obviously, the effective energy barrier is larger than the real one, which is  $\Delta E = 4$  in our example. Moreover,  $\Delta E_{eff}$  is larger for the valley #2 than for #1. This reflects that the system can leave the saddle cluster easier in direction to #2, because there are more exit connections.

In summary, we have shown that the dynamics of spin glasses is related to the microscopic structure of the energy landscape. The characteristic shape of the correlation function and the slow dynamics are caused by the restricted

Table 1

The values of  $q_{pl}$  obtained from the simulations (Fig. 4) and calculation (Eq. (3))

	Fig. 4	Eq. (3)
$q_{pl}$ (#1)	$0.947 \pm 0.004$	0.936
$q_{pl}$ (#2)	$0.932 \pm 0.004$	0.924
$\Delta q_{pl}$	$0.015 \pm 0.004$	0.012

connectivity of clusters and valleys and their internal profiles. Our results are obtained for one particular random set  $\{J_{ij}\}$ . Simulations using different sets confirm that our conclusions are not affected by the choice of  $\{J_{ij}\}$ .

## Acknowledgements

The authors wish to thank A. Heuer for valuable discussions. This work is supported by Graduiertenkolleg “Struktur- und Korrelationeffekte in Festkörpern”.

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